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$d_{x^2-y^2}$ pairing in the generalized Hubbard square-lattice model

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Abstract

The pairing between holes in a square lattice and the two-particle wave-function symmetry are studied within a generalized Hubbard model. The key participation of the next-nearest-neighbor correlated-hopping interaction in the appearance of *d*-wave two-hole ground state is found, which is enhanced by the on-site repulsive Coulomb interaction. There is a clear pairing asymmetry between electrons and holes, where the hole pairing occurs in a realistic regime of interactions. The two-particle states are analyzed by looking at the binding energy, the coherence length, and the effective mass of the pairs. Finally, the case of a hole-singlet in an antiferromagnetic background is also studied. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Since the discovery of high-Tc anisotropic cuprate superconductors, the two-dimensional Hubbard model has been extensively studied, due to its simplicity and emphasis on the local electron–electron correlation which is highly related to the short coherence length observed in these materials [1]. There is a general consensus that the singlets are formed by holes (instead of electrons) and they are mainly restricted to move on the CuO_2 planes. To describe the electron and hole dynamics on these planes, three-band Hubbard models have been proposed [2]. However, these models can be reduced into a single-band ones [3], and the electronic states close to the Fermi energy could be reasonably well described by a square-lattice single-band tight-binding model with a next-nearest-neighbor hopping $t' = 0.45t_0$ [4], where t_0 is the nearest-neighbor hopping parameter.

During the last six years, experimental evidence has shown that there is a condensate of pairs with $d_{x^2-y^2}$ symmetry in several cuprate superconductors [5,6,7]. Numerical studies performed in *t–J* model indicate a dominant *d*-superconducting channel [2], in spite of no long-range *d*-wave superconducting correlation has been found for $J/t \leq 0.5$ [8]. The $d_{x^2-y^2}$ pairing correlation is also observed in a negative nearest-neighbor interaction Hubbard model [9,10] and within a Hubbard like model containing a three-body interaction term [11,12,13]. However, only extended *s*-symmetry pairing has been found within the usual generalized Hubbard models [14], in which a correlated hopping between nearest-neighbors (Δt) is included. In this paper, we consider a generalized single-band Hubbard model without attractive density–density interactions, in which hopping (t') and correlated hopping interaction (Δt_3) between next-nearest-neighbors are considered. We analyze the importance of the correlated hopping interaction Δt_3 in the formation of $d_{x^2-y^2}$ pairing ground-state, in spite of its apparently small strength in comparison with direct Coulomb interactions.

The present paper is organized as follows. Section II contains a brief description of the generalized Hubbard Hamiltonian and the mapping method. In Section III, the two-hole ground-state phase diagram is analyzed, where a *d*-channel pairing zone is observed. In Section IV the case of a hole singlet in an antiferromagnet is investigated. Properties of $d_{x^2-y^2}$ pairing states, such as their binding energy, coherence length and effective mass, are reported. Finally, some conclusions are given in Section V.

2. The model

The original Hubbard model considers only the on-site

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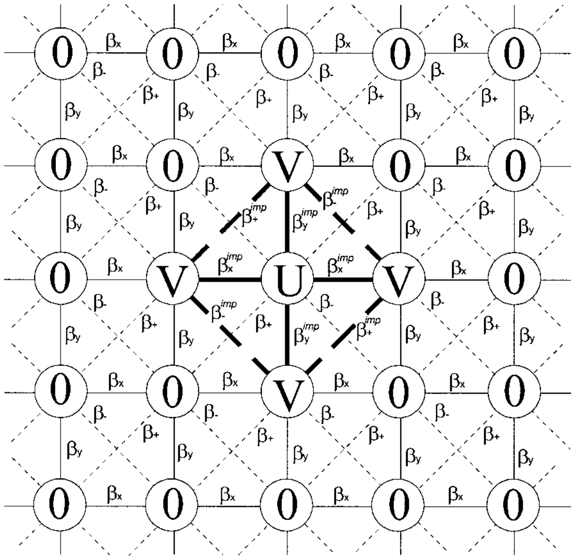

Fig. 1. Schematic representation of the mapped states (circles) of two particles in a square lattice. Their self-energies are shown inside circles, and the hopping strengths between them $\beta_{x(y)}$, $\beta_{\pm}$, $\beta_{x(y)}^{imp}$, and $\beta_{\pm}^{imp}$ are indicated respectively by thin solid, thin dashed, thick solid, and thick dashed lines.

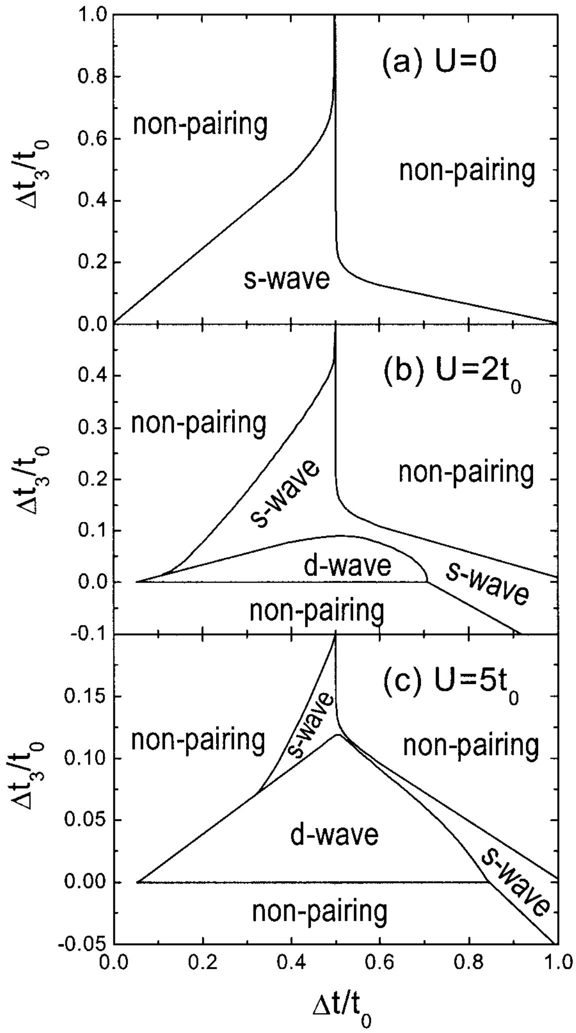

Fig. 2. Hole–singlet ground-state phase diagrams of the generalized Hubbard model with $V = 0$, $t_0' = 0.45t_0$, and (a) $U = 0$, (b) $U = 2t_0$, and (c) $U = 5t_0$.

Coulomb interaction (U), since it is the largest term. However, the addition of a nearest-neighbor Coulomb repulsion (V) allows, for instance, to describe the competition between the charge and spin density waves [17]. Furthermore, the introduction of a nearest-neighbor correlated-hopping interaction (Δt) has shown an enhanced hole-superconductivity without negative U and V [18]. In this paper, we consider a generalized Hubbard model that includes additionally a next-nearest-neighbor correlated hopping interaction (Δt_3). Certainly, all these interactions are present in a real solid, even their contributions are very different, for example, for 3d electrons in transition metals U, V, Δt, and Δt_3 are typically about 20, 3, 0.5, and 0.1 eV, respectively [19,20]. In general, the single s-band generalized Hubbard Hamiltonian can be written as

$$H = -t_0 \sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} - t_0' \sum_{\langle\langle i,j\rangle\rangle,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j + \Delta t \sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{\langle i,l\rangle,\langle j,l\rangle,\langle\langle i,j\rangle\rangle,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} n_l, \quad (1)$$

where $c_{i,\sigma}^{+}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ *or* $\uparrow$ at site i, $n_{i,\sigma} = c_{i,\sigma}^{+} c_{i,\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote respectively the nearest-neighbor and the next-nearest-neighbor sites. In this case, t_0 and t'_0 are positive quantities. When an electron–hole transformation is made in Eq. (1), i.e., electron operators are mapped onto holes via $c_{i,\sigma}^{+} \rightarrow h_{i,\sigma}$, the Hamiltonian becomes:

$$H = (U + 2ZV)(N_s - \sum_{i,\sigma} n_{i,\sigma}^h) + (t_0 - 2\Delta t) \sum_{\langle i,j\rangle,\sigma} h_{i,\sigma}^{+} h_{j,\sigma} + (t_0' - 4\Delta t_3) \sum_{\langle\langle i,j\rangle\rangle,\sigma} h_{i,\sigma}^{+} h_{j,\sigma} + U \sum_i n_{i,\uparrow}^h n_{i,\downarrow}^h + \frac{V}{2} \sum_{\langle i,j\rangle} n_i^h n_j^h + \Delta t \sum_{\langle i,j\rangle,\sigma} h_{i,\sigma}^{+} h_{j,\sigma} (n_{i,-\sigma}^h + n_{j,-\sigma}^h) + \Delta t_3 \sum_{\langle i,l\rangle,\langle j,l\rangle,\langle\langle i,j\rangle\rangle,\sigma} h_{i,\sigma}^{+} h_{j,\sigma} n_l^h, \quad (2)$$

where $n_{i,\sigma}^h = h_{i,\sigma}^{+} h_{i,\sigma}$, $n_i^h = n_{i,\uparrow}^h + n_{i,\downarrow}^h$, N_s is the total number of sites, and Z is the lattice coordination number. The first term in Eq. (2) only contributes to a shift of the total

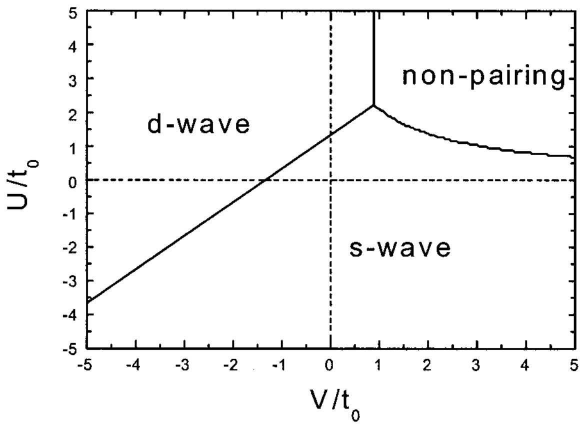

Fig. 3. Hole–singlet ground-state phase diagram in the U–V space, for $t'_0 = 0.45t_0$, $\Delta t = 0.5t_0$ and $\Delta t_3 = 0.25t'_0$.

energy and then, the holes also interact via a generalized Hubbard model but with effective hopping parameters $t = t_0 - 2\Delta t$ and $t' = t'_0 - 4\Delta t_3$, instead of $-t_0$ and $-t'_0$ for electrons.

When the second-neighbor correlated-hopping interaction is introduced, the previously developed mapping method [21] should be modified. For the case of two holes in a square lattice, as shown in Fig. 1, the projected hopping parameters β_x, β_y, $\beta_\pm$, β_x^{imp}, β_y^{imp}, and $\beta_\pm^{imp}$ are respectively given by $2t\cos(K_x a/2)$, $2t\cos(K_y a/2)$, $2t'\cos([K_x \pm K_y]a/2)$, $2t_{imp}\cos(K_x a/2)$, $2t_{imp}\cos(K_y a/2)$, and $2t_3\cos([K_x \pm K_y]a/2)$, where $t_{imp} = t + \Delta t$, $t_3 = t' + \Delta t_3$, (K_x, K_y) is the wave vector of the center of mass of the pair and a is the lattice constant. Notice that the projected hopping strengths, β_x^{imp}, β_y^{imp}, and $\beta_\pm^{imp}$, between "impurity states" (with self-energies U or V) are enhanced by adding respectively Δt, Δt, and Δt_3, since the correlated hopping interactions have contributions only on single-particle hopping between sites close to those occupied by the other particle.

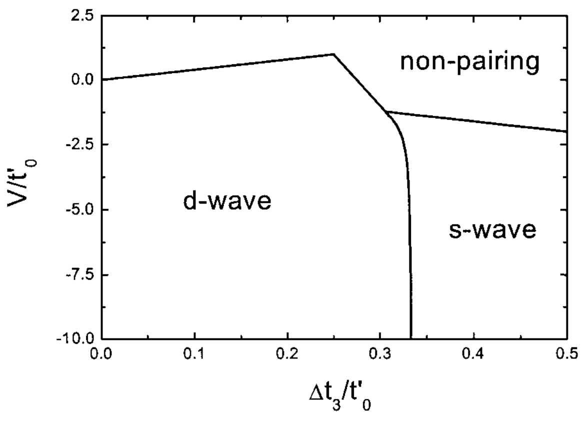

Fig. 4. Ground-state phase diagram of a hole singlet in an antiferromagnet for arbitrary U and Δt.

3. Hole pairing

The pairing between electrons with $U = V = \Delta t_3 = 0$ requires $\Delta t > 2t_0$ for one- and two-dimensional systems [20], which clearly exceeds estimated values of Δt [18], and then only the pairing of holes will be analyzed in this paper in detail. The hole-singlet ground-state phase diagrams shown in Figs 2(a), 2(b), and 2(c) are calculated, respectively, for $U = 0$, $U = 2t_0$, and $U = 5t_0$, all with $V = 0$ and $t'_0 = 0.45t_0$ as suggested by J. Yu, et al. [4]. The numerical calculations are performed in a truncated square lattice, as shown in Fig. 1, of 2401 projected two-particle states. The projected lattice sizes for numerical calculation are chosen as the minimum size so that the physical quantities have no important variation with the lattice size. Note that for $U = 0$ there is no d-symmetry pairing, and as the on-site Coulomb repulsion U increases the $d_{x^2-y^2}$ pairing zone is enlarged. For $U = 10t_0$ the s-wave pairing is essentially avoided. It is some what expected, since the on-site repulsion U inhibits the formation of s-symmetry pairs and does not affect the d ones, therefore it favors the formation of $d_{x^2-y^2}$-pairing ground state. Furthermore, the $d_{x^2-y^2}$ pairing requires that $\Delta t_3 > 0$, regardless of how small it is, which is in agreement with the fact that the correlated hopping Δt alone can give rise only to extended s-wave pairing [14].

The effects of Coulomb interactions U and V on the hole-pairing process are shown in Fig. 3 for $t'_0 = 0.45t_0$, $\Delta t = 0.5t_0$ and $\Delta t_3 = 0.25t'_0$. Notice that for negative V, pairing is essentially in the d-wave channel, as observed previously [9,10]. The phase-transition lines between d-wave and non-pairing, between s-wave and non-pairing, and between d-wave and s-wave regions are respectively found at $V = 4\Delta t_3$, $U = 4t_0^2/(V + 2t'_0)$, and $U = V + t_0^2/t'_0 - 2t'_0$, since for $\Delta t = 0.5t_0$ and $\Delta t_3 = 0.25t'_0$ the mapped lattice (see Fig. 1) is reduced into a molecule of 5 sites whose self-energies are U and V, and then analytical results are obtained. For Δt and Δt_3 being around $0.5t_0$ and $0.25t'_0$, respectively, the general feature of the U–V phase diagrams is essentially the same as Fig. 3.

4. Hole singlets in an antiferromagnet

In this section, we consider a half-filled single-band square lattice, i.e., one electron per site, where an antiferromagnetic long-range order is found for almost all values of the Coulomb repulsion U [15,16]. In this staggered ordered spin background, holes tend to move within the same sublattice to avoid distorting the spin order. Hence, as a first approximation we assume that the antiferromagnetic background remains static when a hole singlet is introduced, although there is evidence that the antiferromagnetic order

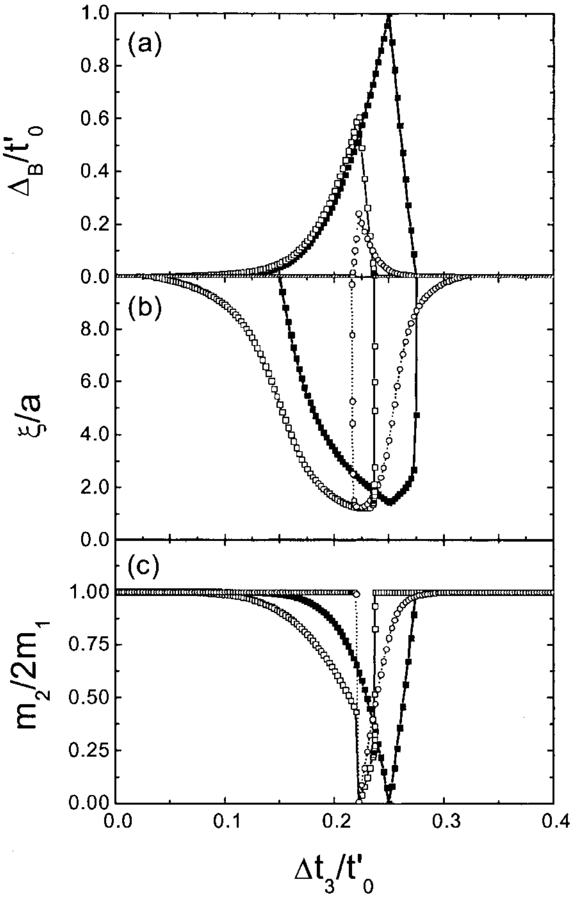

Fig. 5. (a) The binding energy, (b) the coherence length, and (c) the effective mass of *s*-channel (open circles) and *d*-channel (open squares) hole singlets for $U = 5t_0$, $V = 0$, $t'_0 = 0.45t_0$, and $\Delta t = 0.45t_0$ in comparison with those of *d*-channel hole singlets in an antiferromagnet (solid squares) for $V = 0$ and arbitrary U and Δt.

is sensitive to the finite-density doping [16]. Therefore, within this approximation, each hole can move only in one of the two sublattices of the system [9]. This is equivalent to remove the sublattice containing the site with self-energy U in Fig. 1, i.e., the terms of $(t_0 - 2\Delta t)$, U and Δt of the Hamiltonian of holes (Eq. 2) have no effects on this pairing process.

In Fig. 4 the ground-state phase diagram of a hole singlet in a static antiferromagnetic background is shown. Notice that the correlation strengths are expressed in units of the next-nearest-neighbor hopping parameter t'_0, instead of t_0, being $t'_0 < t_0$. Furthermore, the *s*-wave ground state requires a large value of Δt_3 and an attractive nearest-neighbor interaction $V < -4\Delta t_3$, and the *d*-wave pairing needs a screened nearest-neighbor interaction $V < 4\Delta t_3$ for $\Delta t_3 < 0.25t'_0$, or $V < -\frac{12\pi+8}{\pi-2}\Delta t_3 + \frac{4\pi}{\pi-2}t'_0$ for $0.25t'_0 \leq \Delta t_3 \leq \frac{\pi}{2\pi+4}t'_0$. Figures 5(a), 5(b) and 5(c) show, respectively, the binding energy (Δ_B), the coherence length (ξ) and the effective mass (m_2) of a *d*-symmetry hole-singlet in an antiferromagnet (solid squares), in comparison with *s*-channel (open circles) and *d*-channel (open squares) without antiferromagnetic background. The binding energy is defined as $\Delta_B = E_2 - 2E_1$, where E_n is the ground-state energy corresponding to the problem of n holes, and the coherence length is calculated using [20,21]

$$\xi = \left(\frac{\sum_r \psi^*(r) r^2 \psi(r)}{\sum_r \psi^*(r)\psi(r)} \right)^{1/2}, \quad (3)$$

where $\psi(r)$ is the two-particle wave-function amplitude and r represents the internal coordinates of the pair. Finally, in order to study the dynamics of the pairs, their effective mass (m_2), calculated from the dispersion curve of the paired ground-state, is analyzed in comparison with the single-hole effective mass of the lowermost state (m_1). From Fig. 5(a) it can be noted that the antiferromagnetic background enhances the *d*-wave pairing. Also, notice that in general a short coherence length is associated to a larger binding energy, as occurred in the BCS theory [22]. However, the *d*-channel pairs in an antiferromagnet, having a larger binding energy in comparison with the *s*-channel ones, do not possess a shorter coherence length around $\Delta t_3 = 0.225t'_0$. This fact could be important since a larger binding energy leads to a higher pair-formation temperature and a longer coherence length could help the condensation of Bose–Einstein [24]. On the other hand, a significant reduction of $m_2/2m_1$ around $t = 2t'$ is observed, because the correlated hopping interactions enhance the mobility of the pairs and the effective mass of single holes (m_1) becomes extremely large in this region, similar to that occurred in generalized Hubbard systems with only a nearest-neighbor correlated hopping [20].

5. Conclusions

In summary, we have studied the hole-pairing symmetry within the generalized Hubbard model, in which a second-neighbor correlated-hopping term is included. In spite of its smaller strength in comparison with other terms of the model, we have found its key participation in the formation of the *d*-channel hole pairs. The single-pair dynamics has been studied by extending a previously developed mapping method. This method has the advantage of giving a clear association between the pairing and the impurity states [20], and provides a new way to analyze the pairing process in randomly disordered systems [25].

No matter how small is the value of the second-neighbor correlated hopping, a *d*-symmetry ground-state region is found for $U > 0$, and such region grows with U. It is worth mentioning that the *d*-channel pairing is sensitive to the next-nearest neighbor electron–electron interaction.

However, some effective one-band Hubbard models that describe the low-energy physics of cuprate superconductors usually take $V = 0$ [23]. On the other hand, a larger binding energy and longer coherence length of the d-channel pairs in an antiferromagnetic background have been obtained around $\Delta t_3 = 0.225t'_0$, as compared with the s-channel's ones, which could be important for the d-wave superconductivity in the crossover model [24]. Furthermore, the effective mass of paired holes shows a significant reduction in comparison with that of single holes, since the correlated hopping interaction introduces a new transport mechanism of pairs, in which the presence of one hole enhances the hopping of the other, even though in the regions the mobility of single holes is almost null. This fact could help the Bose–Einstein condensation of these hole singlets, when a small interplane coupling is turned on; contrary to the case of the negative U or V, where the effective mass of hole singlets increases when the pairing interactions grow [26]. Finally, the present study has shown that terms usually ignored in the Hubbard model could be relevant in certain phenomena, such as the d-channel pairing.

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References

[1] R. Micnas, J. Ranninger, S. Robaszkiewicz, Rev. Mod. Phys. 62 (1990) 113.
[2] E. Dagotto, Rev. Mod. Phys. 66 (1994) 763.
[3] H.-B. Schuttler, A.J. Fedro, Phys. Rev. B 45 (1992) 7588.
[4] J. Yu, S. Massidda, A.J. Freeman, Physica C 152 (1988) 273.
[5] D.A. Wollman, et al., Phys. Rev. Lett. 71 (1993) 2134.
[6] D.A. Wollman, et al., Phys. Rev. Lett. 74 (1995) 797.
[7] C.C. Tsuei, J.R. Kirtley, Rev. Mod. Phys. 72 (2000) 969.
[8] C.T. Shih, Y.T. Chen, H.Q. Lin, T.K. Lee, Phys. Rev. Lett. 81 (1998) 1294.
[9] A. Nazarenko, A. Moreo, E. Dagotto, J. Riera, Phys. Rev. B 54 (1996) R768.
[10] A.S. Blaer, H.C. Ren, O. Tchernyshyov, Phys. Rev. B 55 (1997) 6035.
[11] L. Arrachea, A.A. Aligia, Phys. Rev. B 59 (1999) 1333.
[12] L. Arrachea, A.A. Aligia, Phys. Rev. B 61 (2000) 9686.
[13] J.E. Hirsch, Phys. Lett. A 136 (1989) 163.
[14] H.Q. Lin, J.E. Hirsch, Phys. Rev. B 35 (1987) 3359.
[15] J.E. Hirsch, S. Tang, Phys. Rev. Lett. 62 (1989) 591.
[16] J.E. Hirsch, Phys. Rev. Lett. 53 (1984) 2327.
[17] F. Marsiglio, J.E. Hirsch, Physica C 171 (1990) 554.
[18] J. Hubbard, Proc. R. Soc. London Ser. A 276 (1963) 238.
[19] J. Appel, M. Grodziki, F. Paulsen, Phys. Rev. B 47 (1993) 2812.
[20] L.A. Pérez, C. Wang, Solid State Commun. 108 (1998) 215.
[21] M. Randeria, J.-M. Duan, L.-Y. Shieh, Phys. Rev. B. 41 (1990) 327.
[22] J. Bardeen, L.N. Cooper, J.R. Schrieffer, Phys. Rev. 108 (1957) 1175.
[23] M.E. Simón, A.A. Aligia, Phys. Rev. B 48 (1993) 7471, and references therein.
[24] M. Randeria, in: A. Griffin (Ed.), Bose-Einstein Condensation, Cambridge University Press, 1995.
[25] R. Oviedo-Roa, C. Wang, O. Navarro, J. Low Temp. Phys. 105 (1996) 651.
[26] L.A. Pérez, C. Wang, Physica B 259-261 (1999) 771.